

Cold & Ultra-cold Neutron Sources R&D

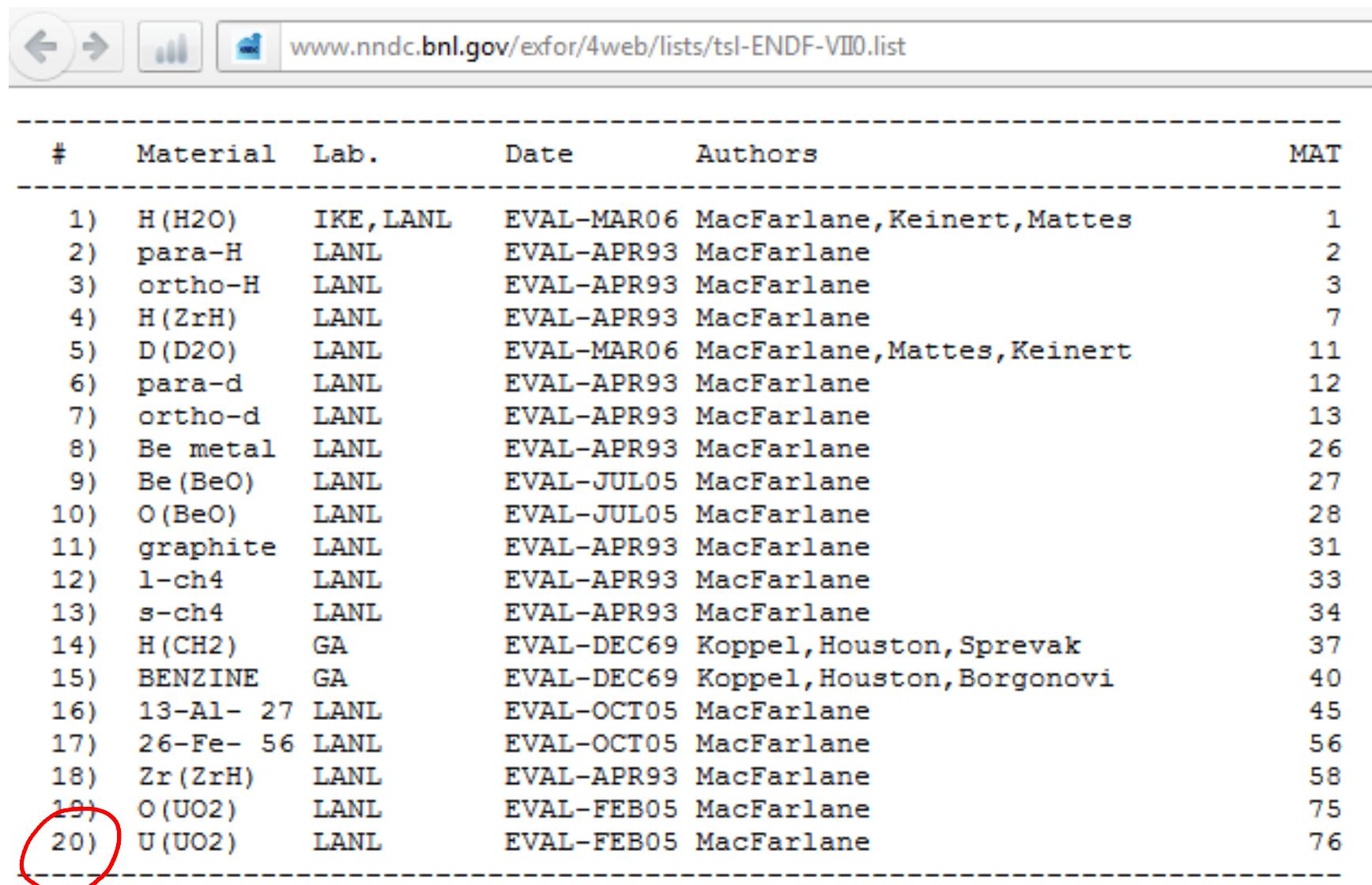
Chen-Yu Liu
Indiana University

Cold Neutron Source Development

- Goal: cool the neutron MB spectrum towards 5K
- Moderator Material
 - Large inelastic scattering (H, D, O)
 - Small neutron absorption (D, O)
- Geometry
 - Enhance efficiency of thermal neutron flux trap (C, D₂O, nano-particles)
 - Enhance efficiency of extraction of moderated cold neutrons (grooved moderator, hybrid moderators)
- High power requirement
 - Cooling 1MW target (sub-cooled He)

} This talk .

Existing Cold Neutron Scattering Kernels



www.nndc.bnl.gov/exfor/4web/lists/tsl-ENDF-VIII.list

#	Material	Lab.	Date	Authors	MAT
1)	H(H ₂ O)	IKE, LANL	EVAL-MAR06	MacFarlane, Keinert, Mattes	1
2)	para-H	LANL	EVAL-APR93	MacFarlane	2
3)	ortho-H	LANL	EVAL-APR93	MacFarlane	3
4)	H(ZrH)	LANL	EVAL-APR93	MacFarlane	7
5)	D(D ₂ O)	LANL	EVAL-MAR06	MacFarlane, Mattes, Keinert	11
6)	para-d	LANL	EVAL-APR93	MacFarlane	12
7)	ortho-d	LANL	EVAL-APR93	MacFarlane	13
8)	Be metal	LANL	EVAL-APR93	MacFarlane	26
9)	Be(BeO)	LANL	EVAL-JUL05	MacFarlane	27
10)	O(BeO)	LANL	EVAL-JUL05	MacFarlane	28
11)	graphite	LANL	EVAL-APR93	MacFarlane	31
12)	l-ch ₄	LANL	EVAL-APR93	MacFarlane	33
13)	s-ch ₄	LANL	EVAL-APR93	MacFarlane	34
14)	H(CH ₂)	GA	EVAL-DEC69	Koppel, Houston, Sprevak	37
15)	BENZINE	GA	EVAL-DEC69	Koppel, Houston, Borgonovi	40
16)	13-Al- 27	LANL	EVAL-OCT05	MacFarlane	45
17)	26-Fe- 56	LANL	EVAL-OCT05	MacFarlane	56
18)	Zr(ZrH)	LANL	EVAL-APR93	MacFarlane	58
19)	O(UO ₂)	LANL	EVAL-FEB05	MacFarlane	75
20)	U(UO ₂)	LANL	EVAL-FEB05	MacFarlane	76

Existing Cold Neutron Scattering Kernels

www.nndc.bnl.gov/exfor/e4explorer.htm

Flexible Database Explorer

Restart Close Config Selection Help About

R-T-L-Q Evaluated data [+Reaction]
T-L-R-Q G Photo-Nuclear Data
T-L-R-Q PHOTO Photo-Atomic Interaction Data
T-L-R-Q DECAY Radioactive Decay Data
T-L-R-Q S/FPY Spontaneous Fission Product Yields
T-L-R-Q N Incident-Neutron Data
T-L-R-Q N/FPY Neutron-Induced Fission Product Yields
T-L-R-Q TSL Thermal Neutron Scattering Data
T-L-R-Q Std Neutron Cross Section Standards
T-L-R-Q E Electro-Atomic Interaction Data
T-L-R-Q P Incident-Proton Data
T-L-R-Q D Incident-Deuteron Data
T-L-R-Q T Incident-Triton Data
T-L-R-Q HE3 Incident-He3 data

Configuration: [Show]
Video demo: [show]
How-to slides: [show]

2012/06/18, 15:40:14, www.nndc.bnl.gov
Flex-DB-Ex - Flexible Database Explorer, v-1.004, 2008/07/09
Created by V.Zerkin, IAEA, 2005-2008

28) SIO2(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
29) U(UO2) (TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
30) U(UO2) (TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
31) MG(TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
32) MG(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
33) AL-27(TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
34) AL-27(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
35) FE-56(TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
36) FE-56(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
37) ZR(ZRH) (TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
38) ZR(ZRH) (TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
39) CA(CAH2) (TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
40) CA(CAH2) (TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
41) U(UO2) (TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
42) U(UO2) (TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
43) U(UC) (TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
44) U(UC) (TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
45) BE-9(TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
46) BE-9(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
47) AL-27(TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
48) AL-27(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12
49) FE-56(TSL, EL), SIG/THS MT=2 MF=7 NSUB=12
50) FE-56(TSL, INL), SIG/THS MT=4 MF=7 NSUB=12

MF7: [SIG/THS] Thermal neutron scattering law data MT4: [N,INL] Production of one neutron in the exit channel
104 ENDF-6 Interpreted ENDF/B-VII.0 Lab=LANL Date=DIST-DEC06

NEW THERMAL NEUTRON SCATTERING FILES FOR ENDF/B-VI RELEASE 2

R. E. MacFarlane

August 24, 1994

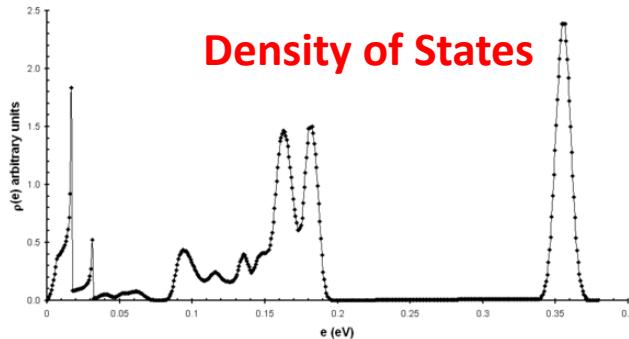
CONTENTS

- Incoherent Elastic (easy)
- Coherent Elastic (OK)
- Incoherent Inelastic (easy)
- Coherent Inelastic (hard!)

I.	INTRODUCTION
II.	THE LEAPR MODULE OF NJOY
A.	Theory
B.	LEAPR Input Instructions
III.	BERYLLIUM METAL
IV.	BERYLLIUM OXIDE
V.	GRAPHITE
VI.	WATER
VII.	ZIRCONIUM HYDRIDE
VIII.	SOLID METHANE
IX.	LIQUID METHANE
X.	LIQUID HYDROGEN
XI.	LIQUID DEUTERIUM
XII.	ACKNOWLEDGMENTS
XIII.	REFERENCES

hcp lattice {
fcc → {
spin }

Cold Neutron Scattering Kernel (using NJOY)



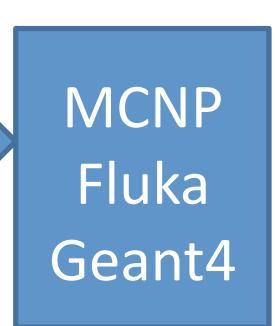
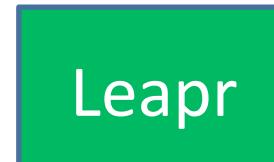
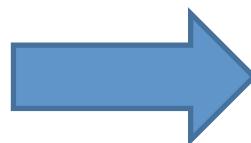
$$\sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} S(\alpha, \beta),$$

$$S_s(\alpha, \beta) = e^{-\alpha \lambda_s} \sum_{n=0}^{\infty} \frac{1}{n!} \alpha^n \text{ Phonon expansion (Incoherent approximation)} \\ \times \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta\hat{t}} \left[\int_{-\infty}^{\infty} P_s(\beta') e^{-\beta'/2} e^{-i\beta'\hat{t}} d\beta' \right]^n d\hat{t}.$$

Other approximations:

Short-Collision-Time Approx., Diffusion & Free-gas translation, Discrete oscillators

$$\sigma_{coh}(E, \mu) = \frac{\sigma_c}{E} \sum_{E_i < E} f_i e^{-4WE_i} \delta(\mu - \mu_i),$$



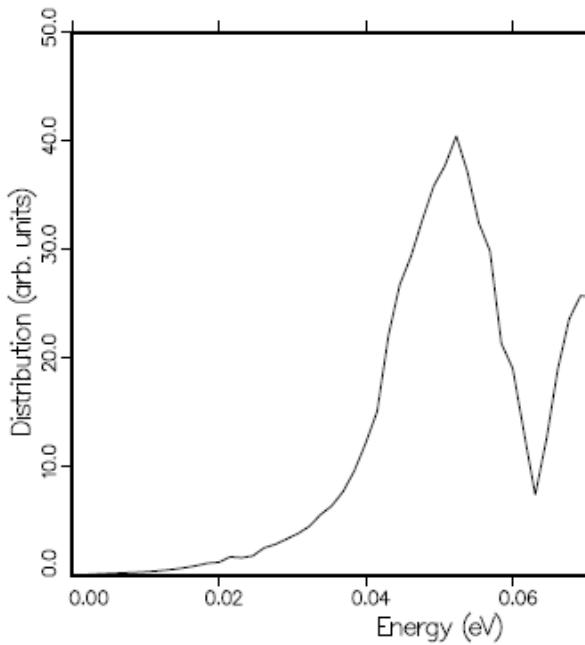
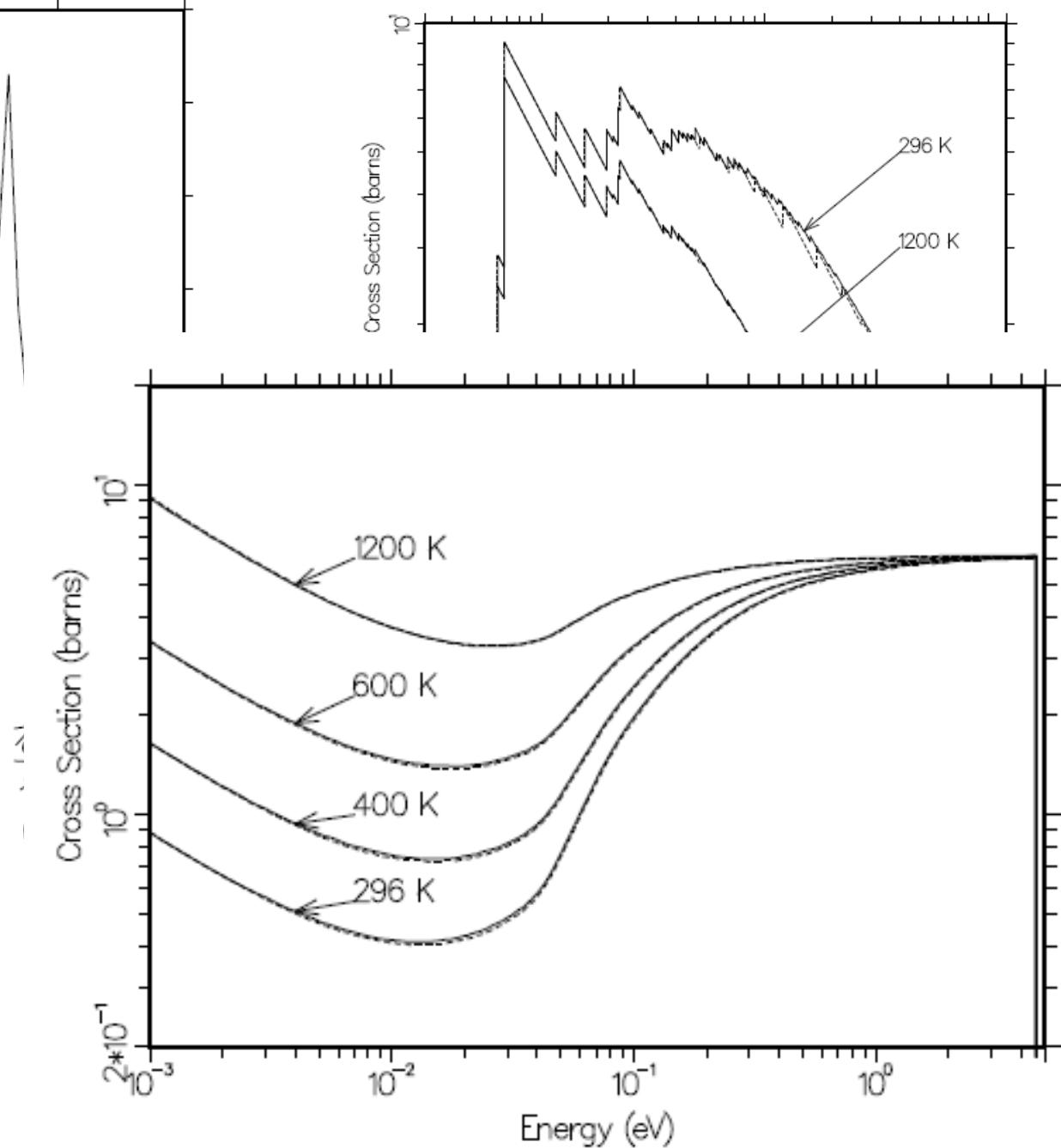
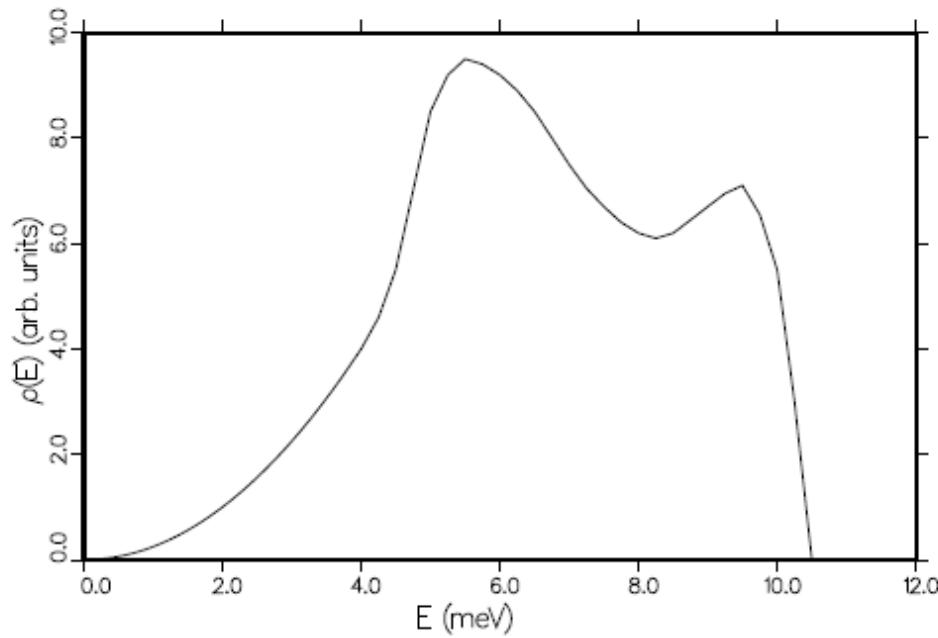


Figure 1: The phonon frequency spectrum $\rho(\omega)$.



- Be
- hcp lattice

Figure 16: Perspective view of the secondary neutron spectra from



Liquid H₂

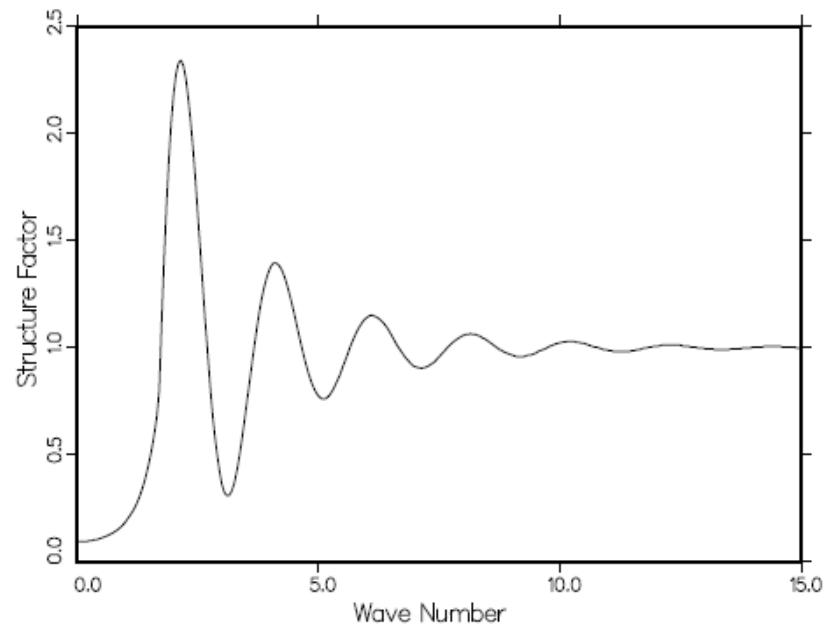
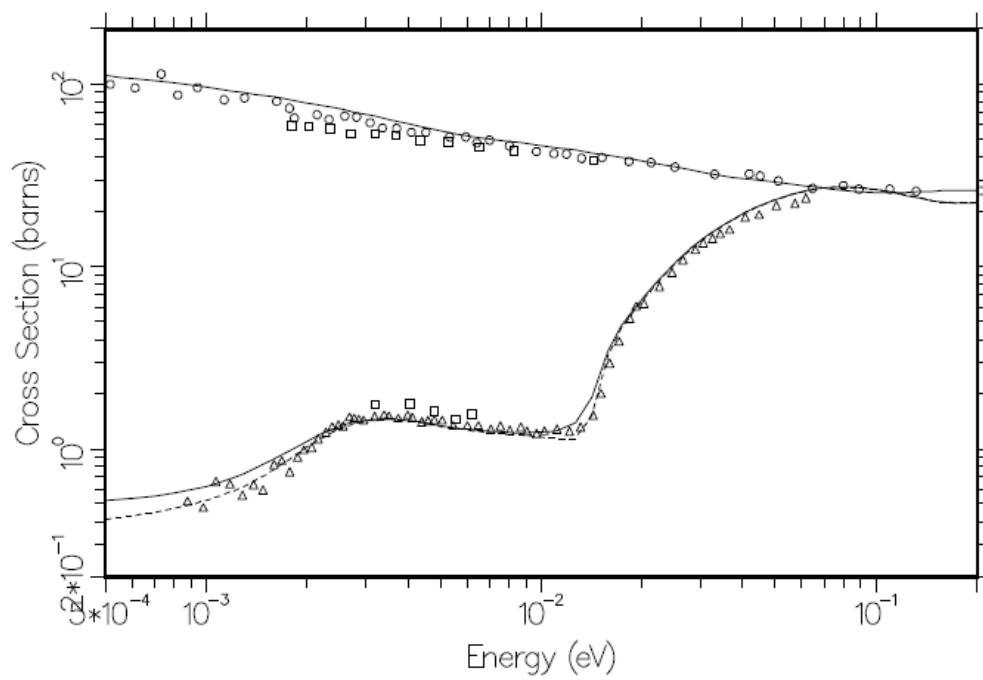
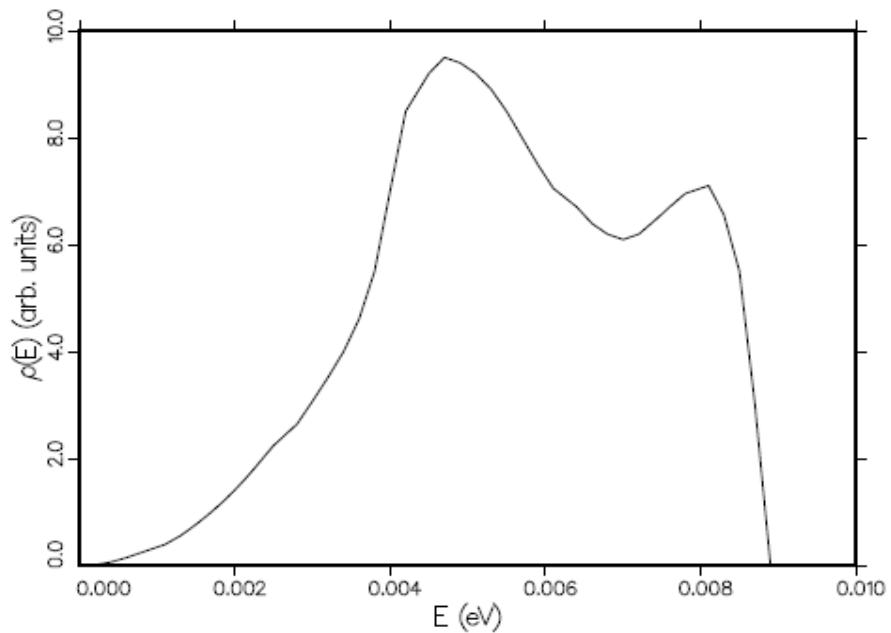


Figure 82: The static structure factor $S(\kappa)$ for liquid hydrogen.



Liquid D₂

Fig
tran

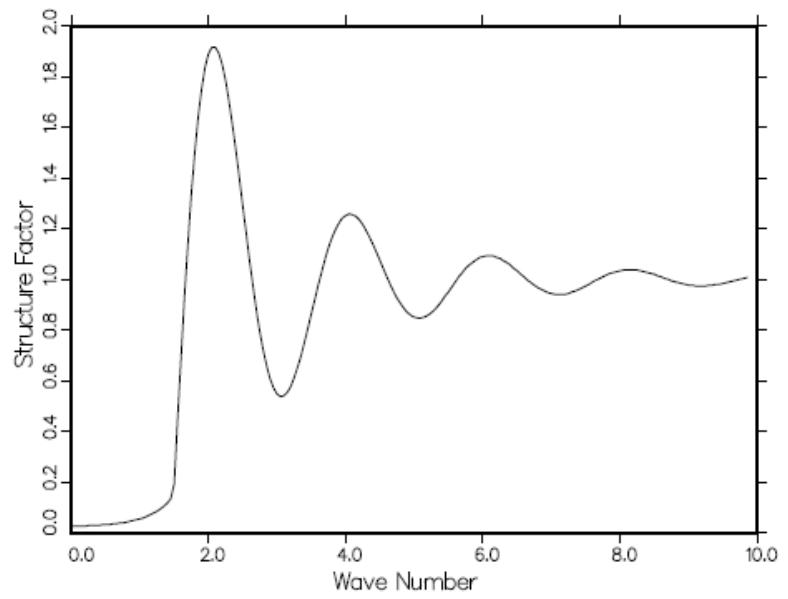
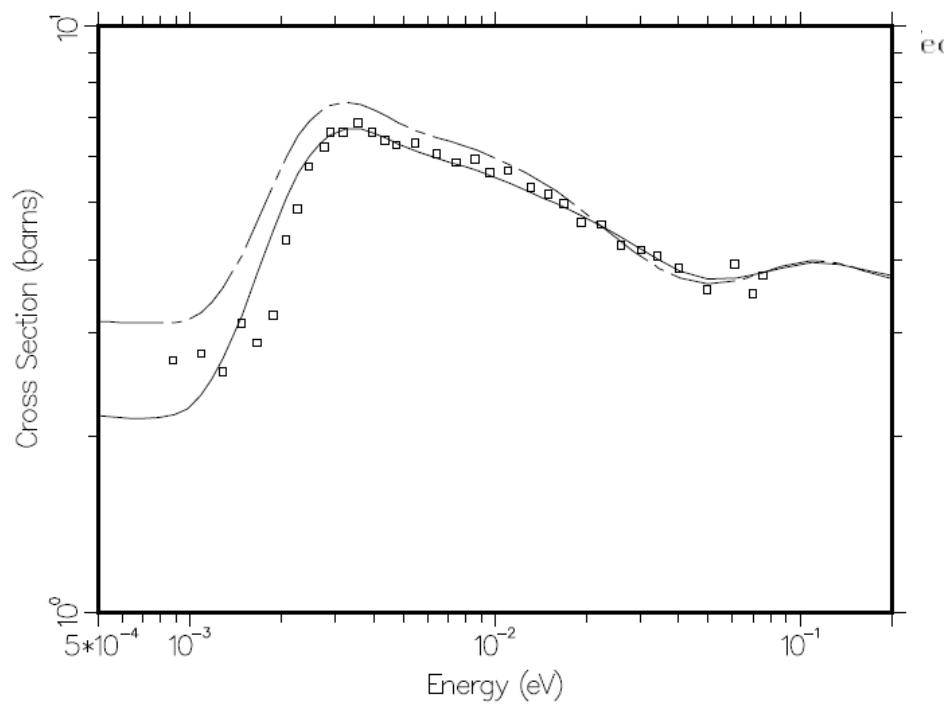
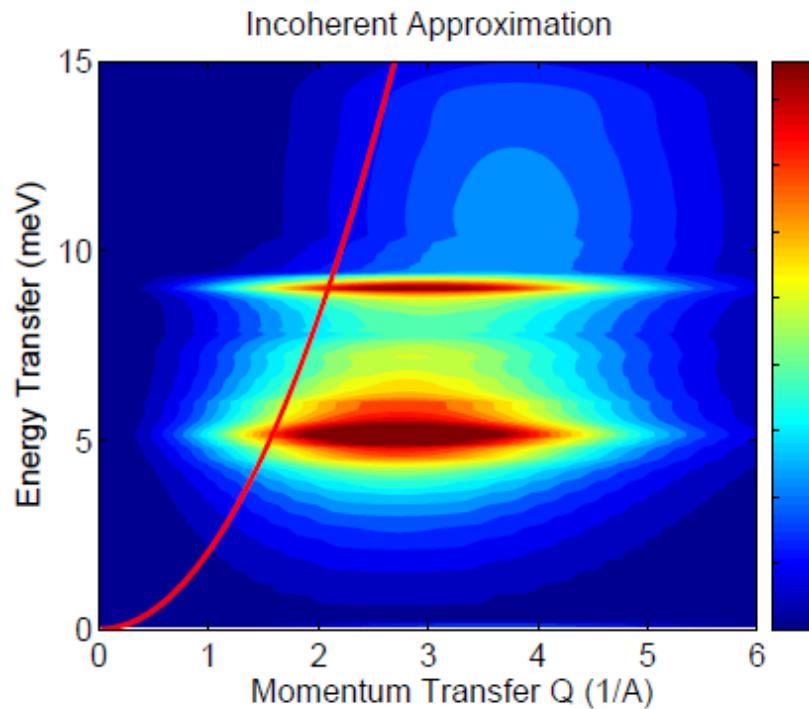


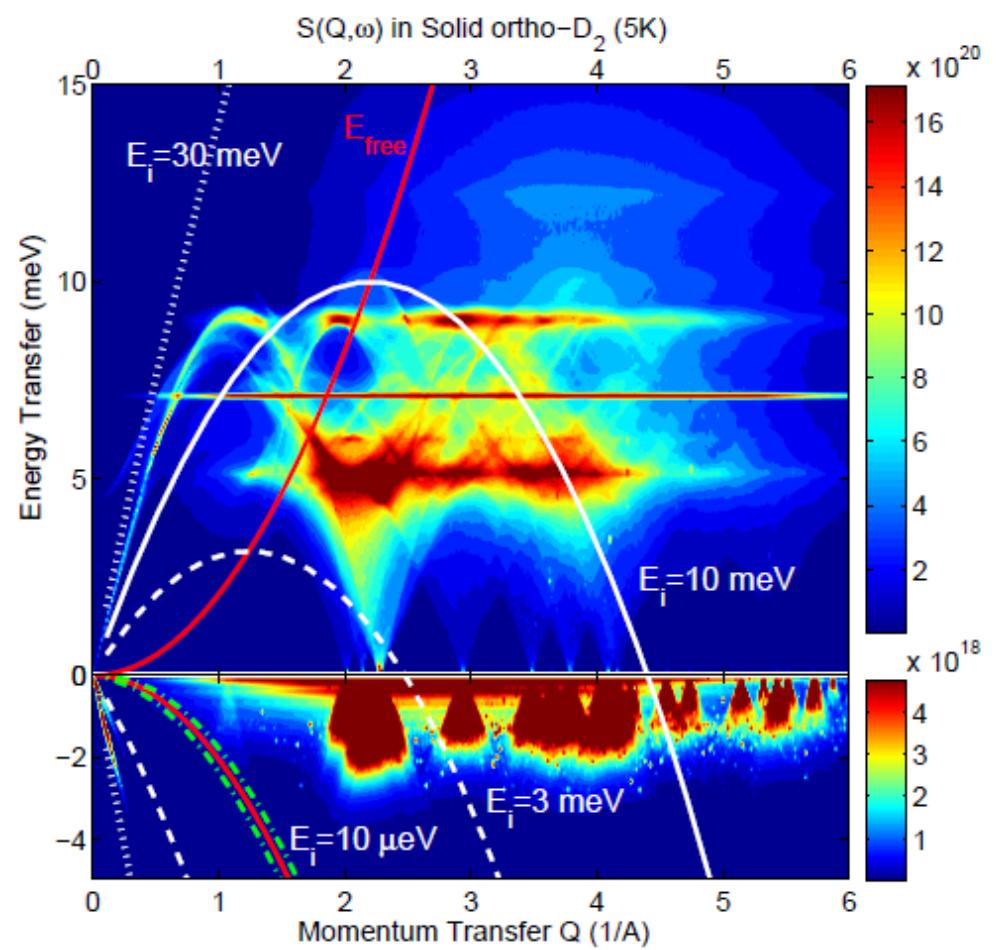
Figure 95: The static structure factor $S(\kappa)$ for liquid deuterium.

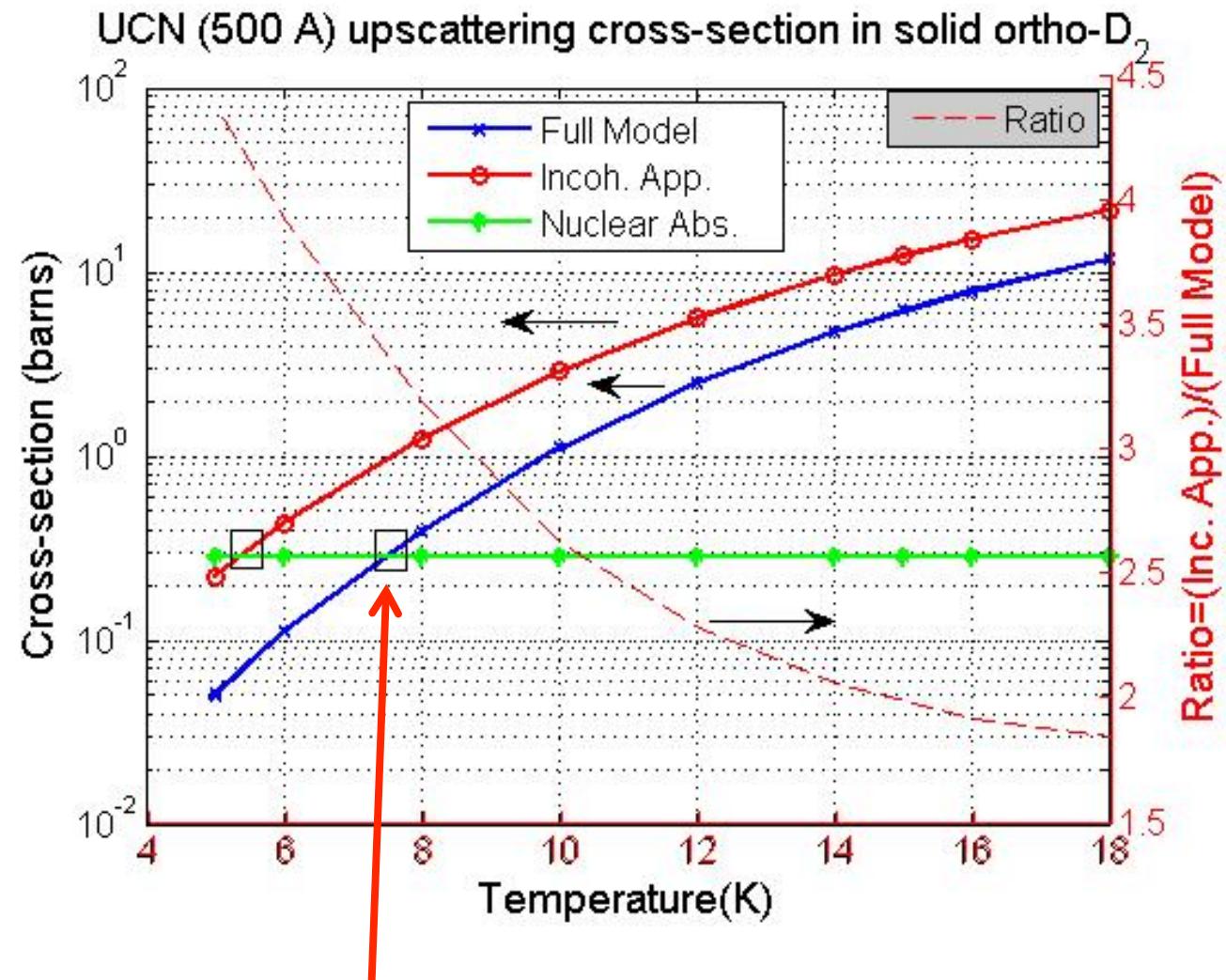
Incoherent Approximation

- Inc. Approx.



Semi-ab initio calculation





Higher saturation temperature!

Solid Oxygen as a UCN Source

$\sigma_{coh} = 4.232$ barn, $\sigma_{inc} = 0$ barn,

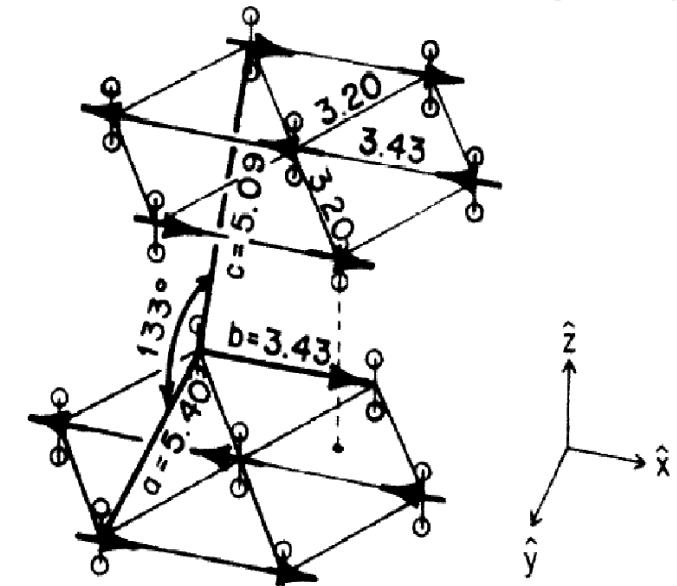
$\sigma_{abs} = 0.0001$ barn

- Electronic spin $S=1$ in O_2 molecules.
- Nuclear spin = 0 in ^{16}O
- Collinear Anti-ferromagnetic in 2-D
 - α -phase, $T < 24K$.

Stephens & Majkrzak, PRB 33, 1 (1986)

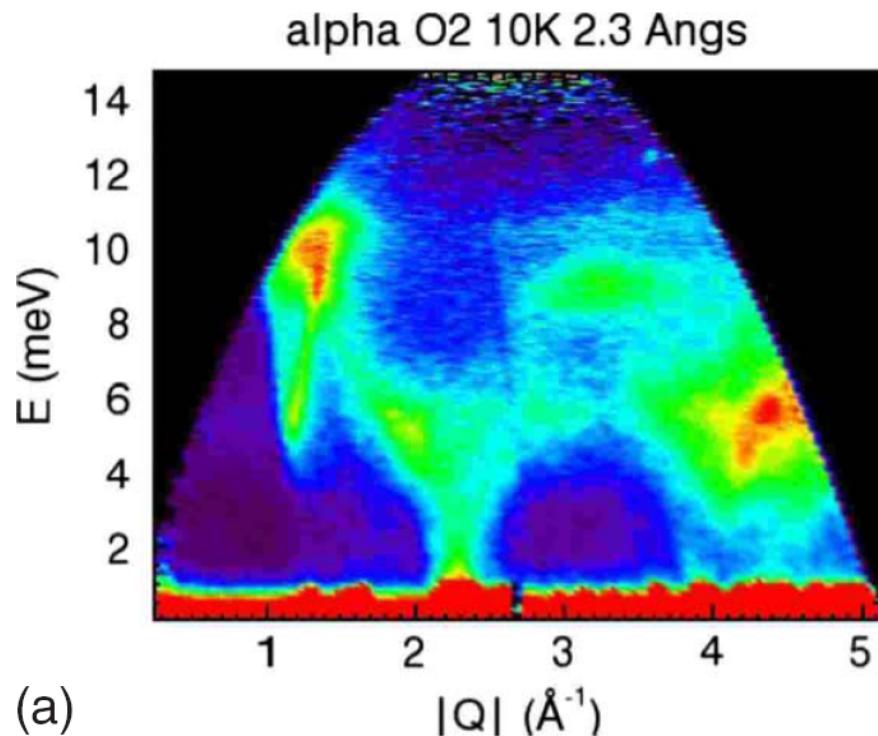
UCN Production in alpha S-O₂

- Produce UCN through magnon excitations.
 - Magnetic scattering length ~ 5.4 fm.
- Null incoherent scattering length.
- Small nuclear absorption probability.



\Rightarrow A very large source possible.

Inelastic neutron scattering data



**Spin self-energy is
very strong along the
direction of spin
alignment!**

Calculations

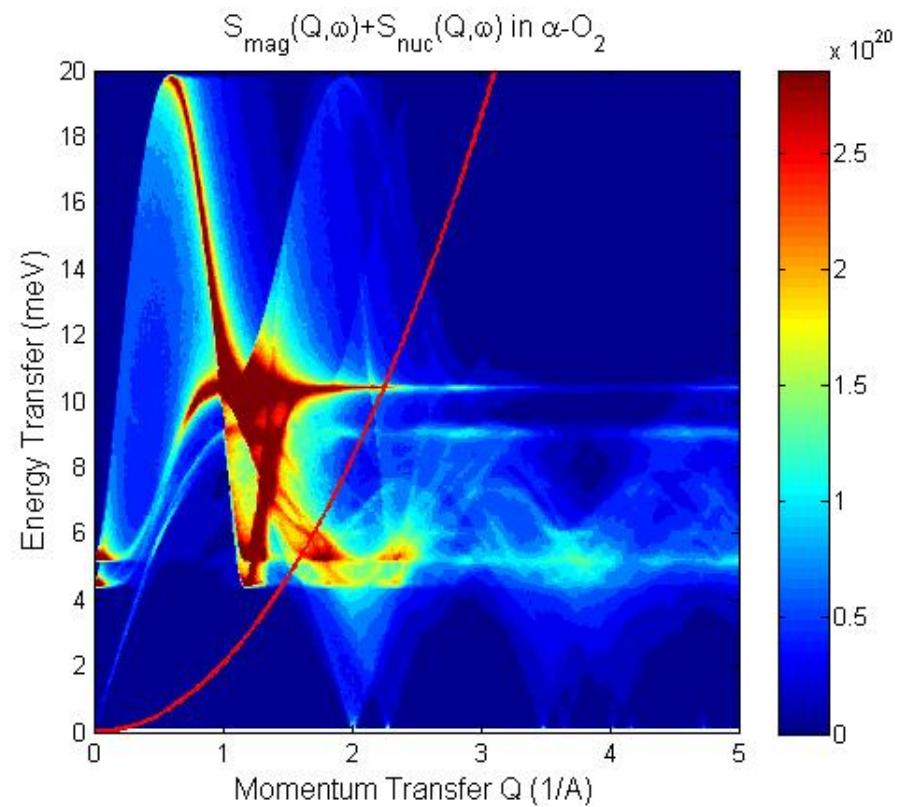
$$H = -2 \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i (-D S_{xi}^2 - D' S_{yi}^2 + D' S_{zi}^2)$$

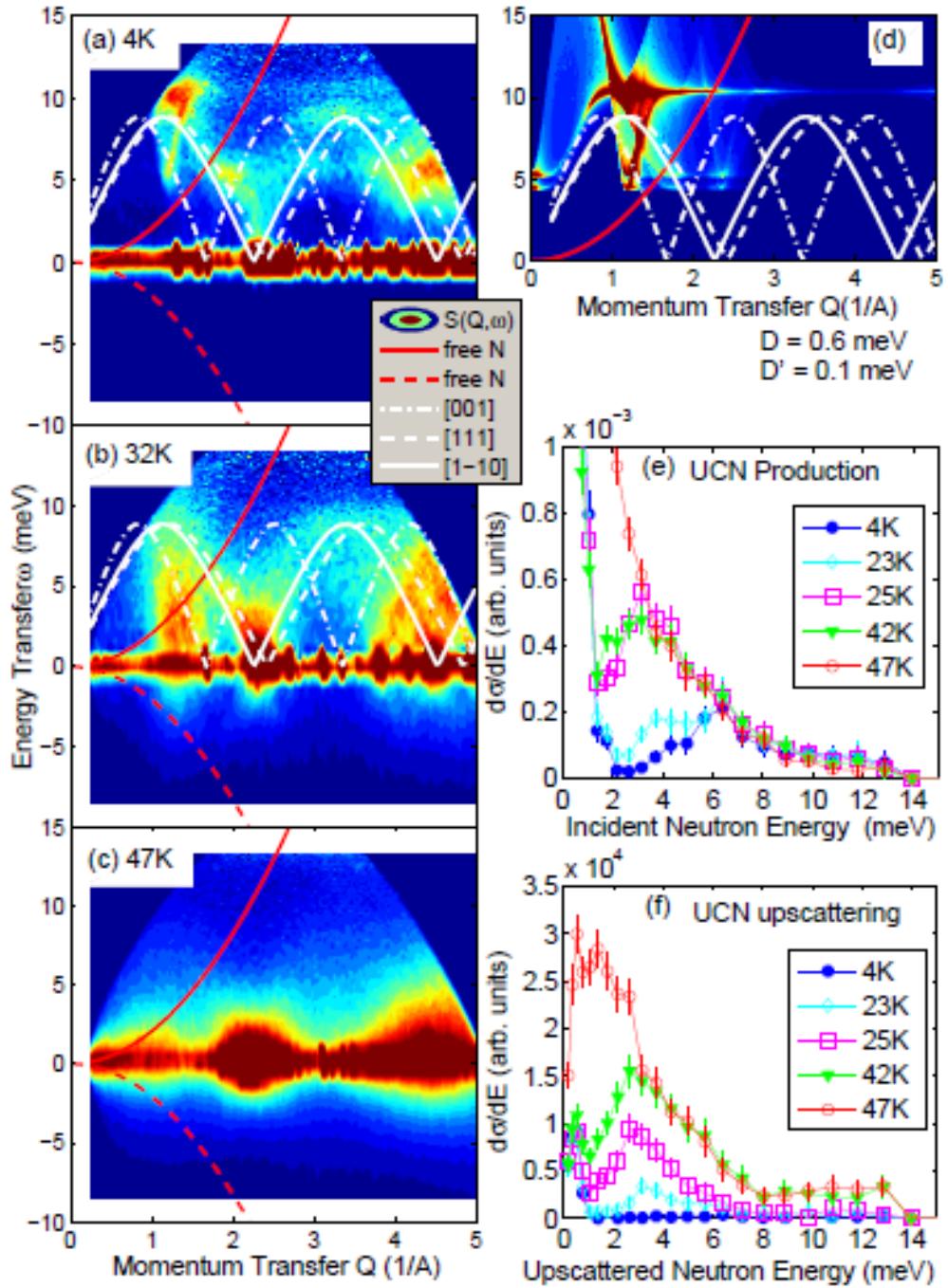
$$J_{nn} = -2.44 \text{ meV}$$

$$J_{nnn} = -1.22 \text{ meV}$$

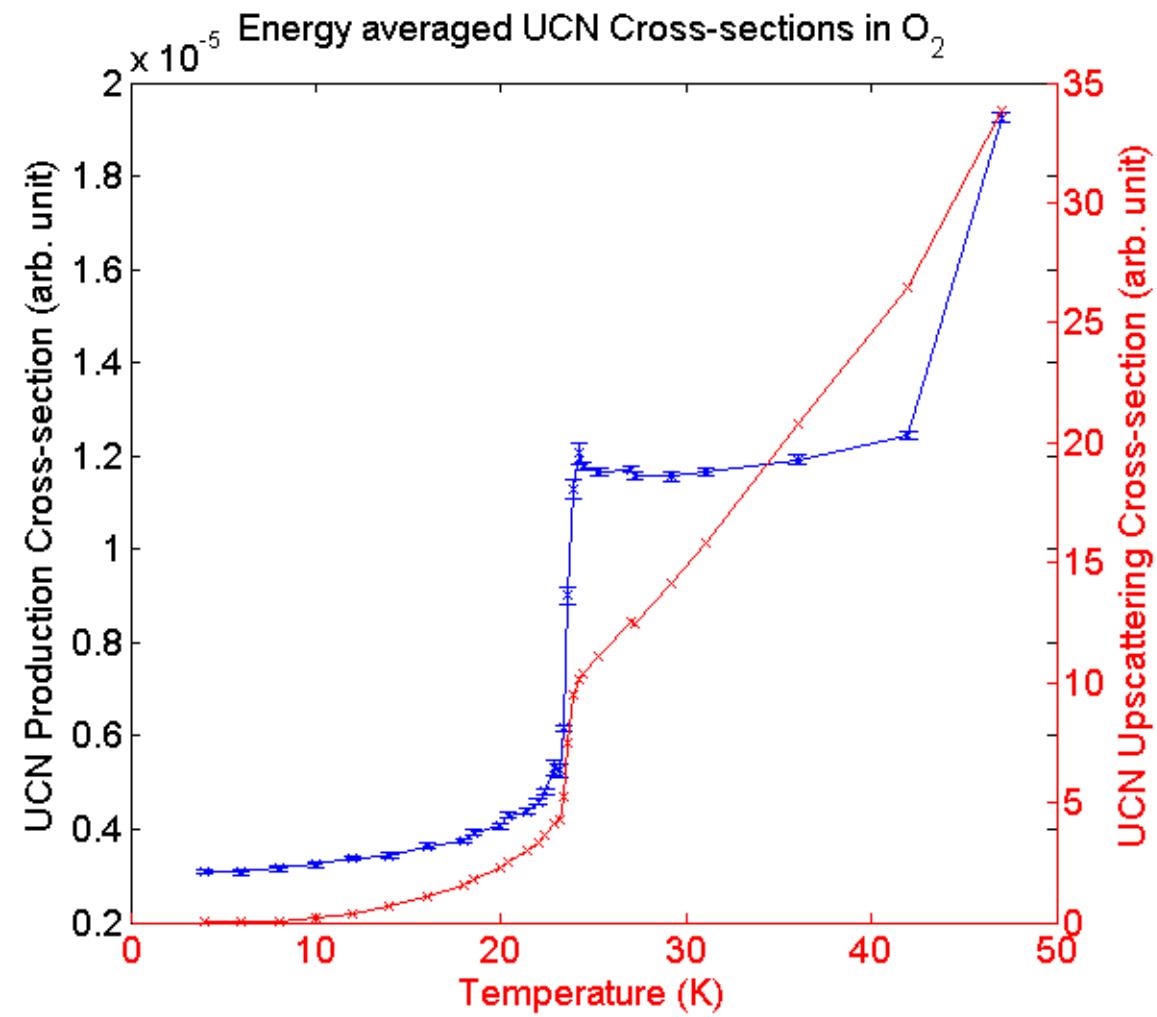
$$D = 0.6 \text{ meV (updated)}$$

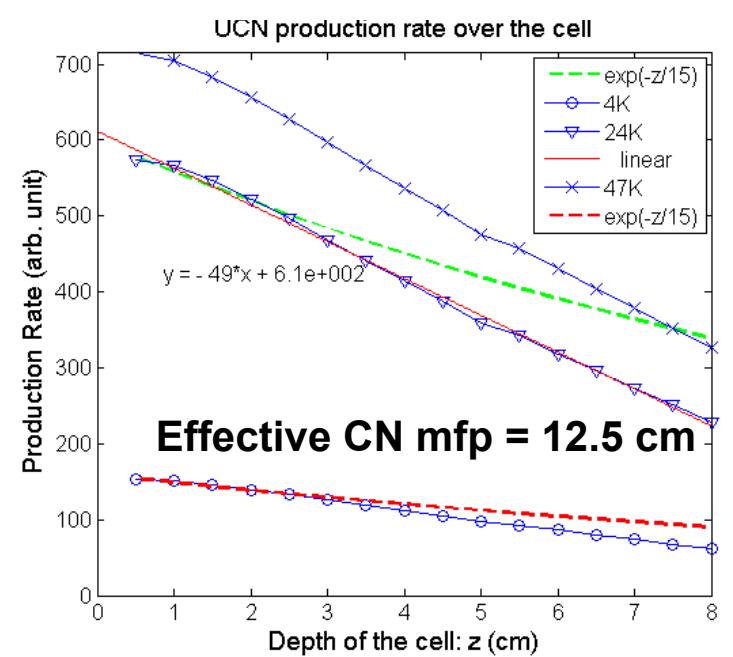
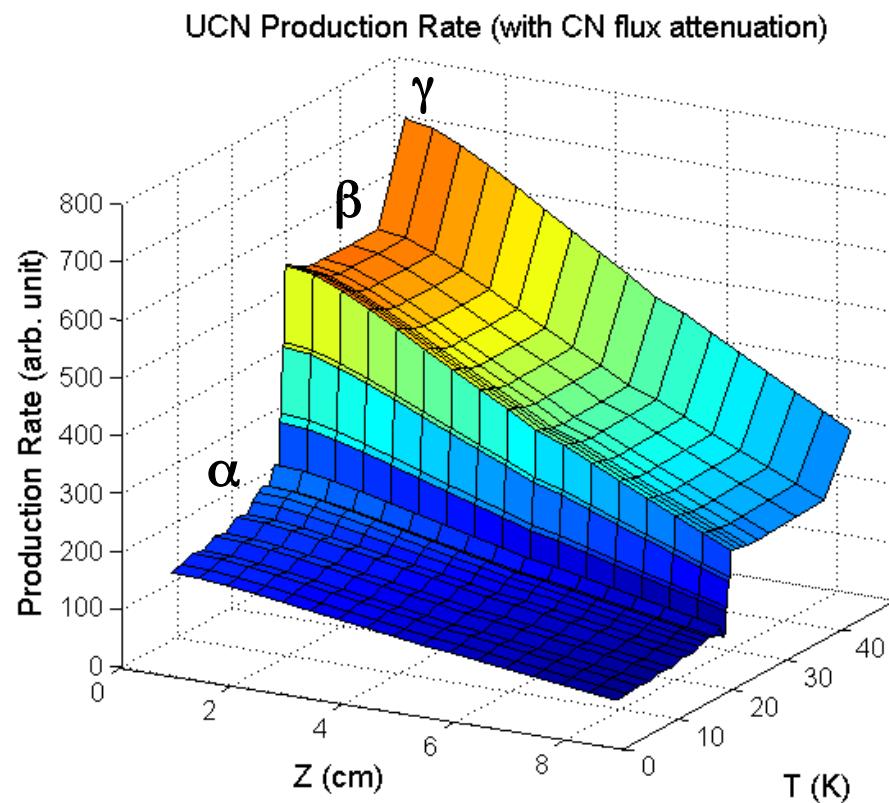
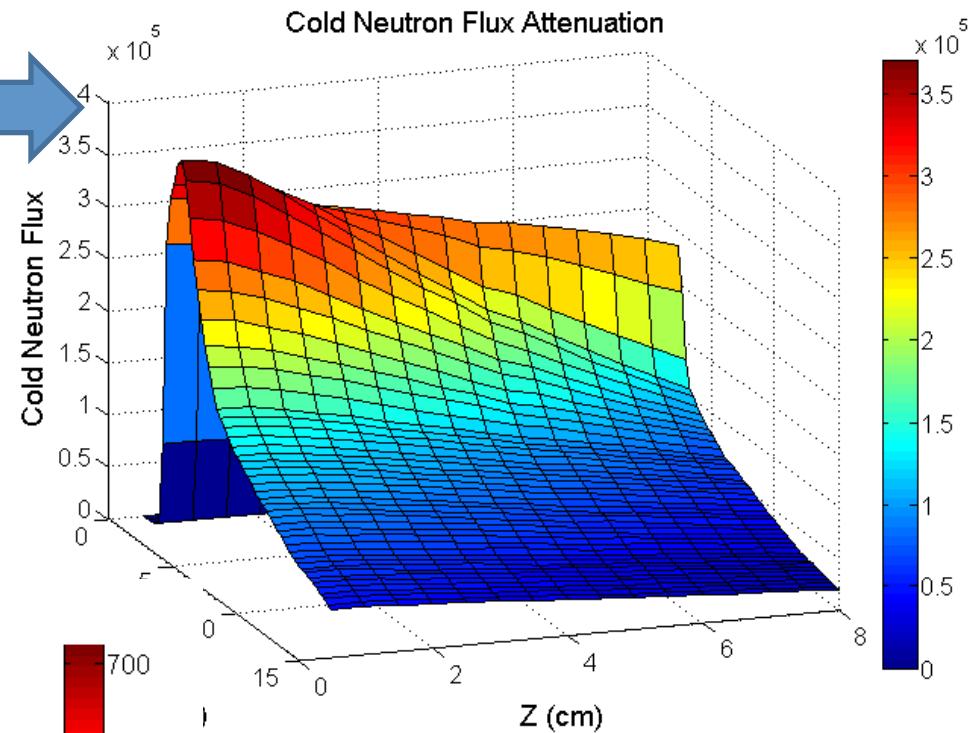
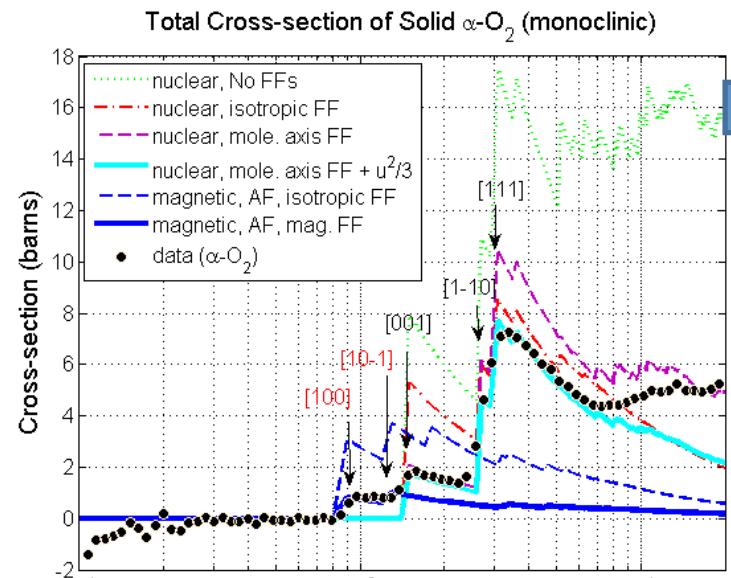
$$D' = 0.1 \text{ meV}$$





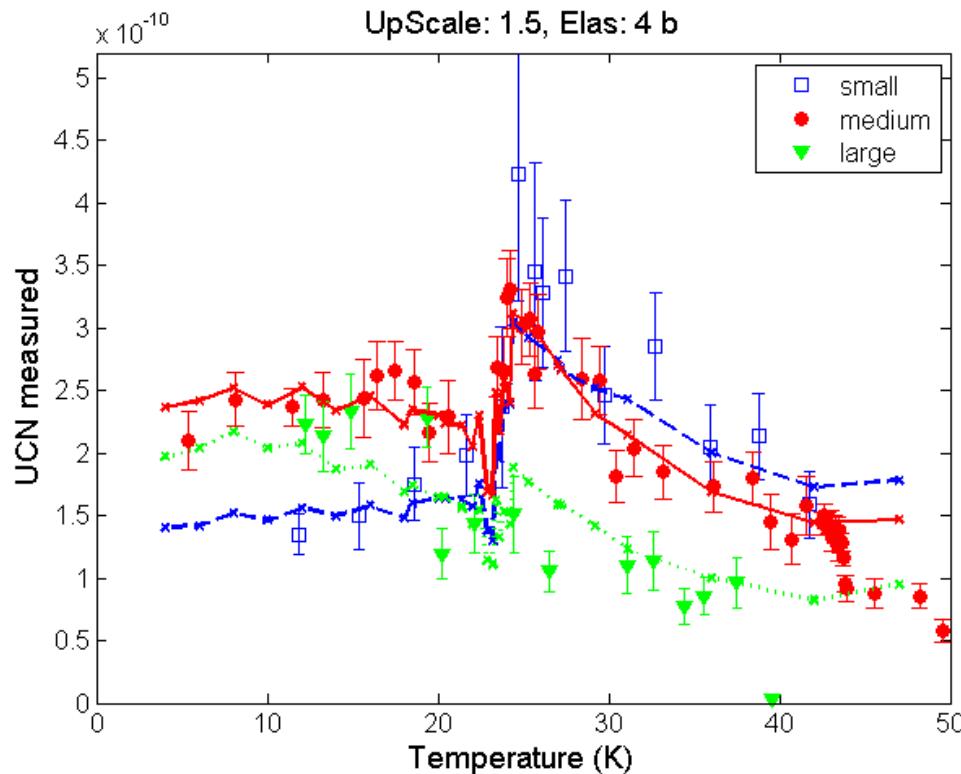
UCN Production & Upscattering Cross Sections



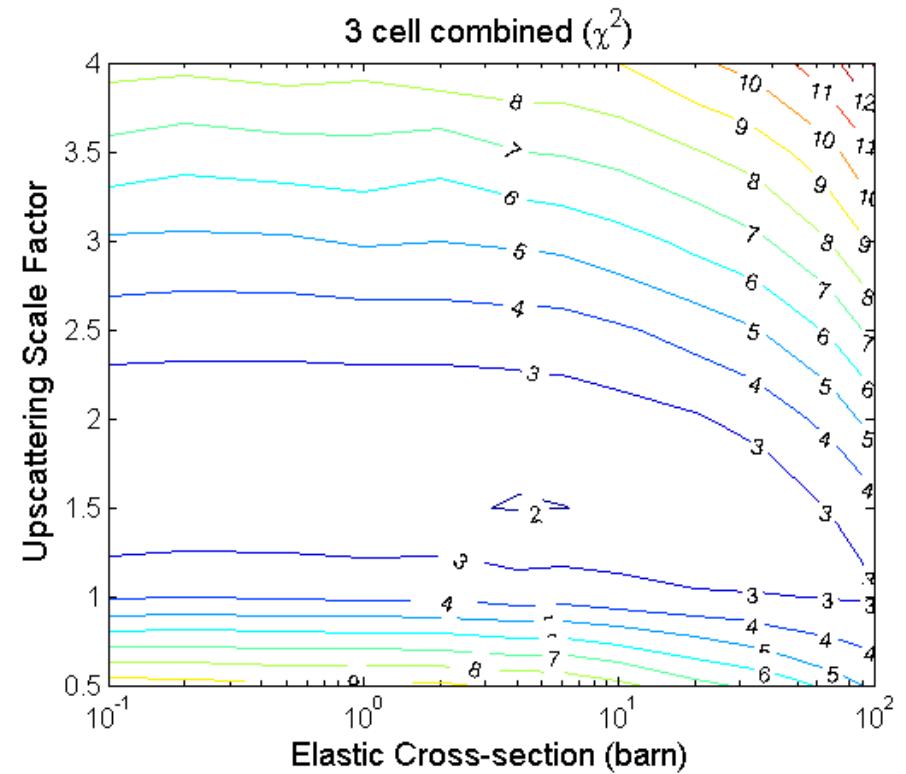


Combined analysis

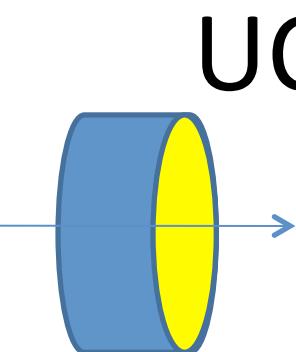
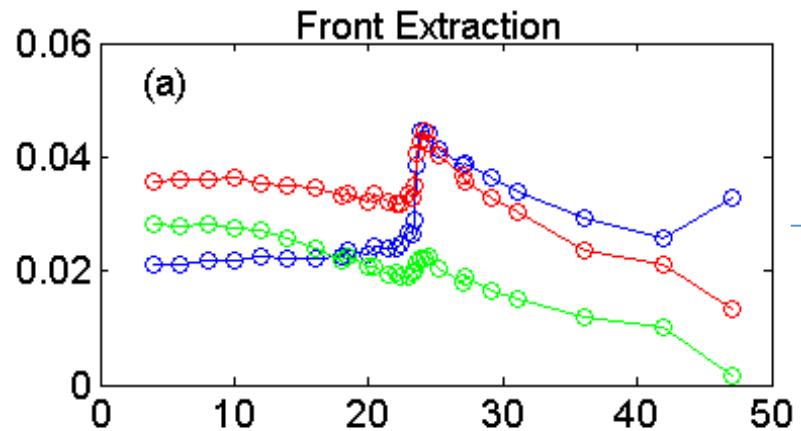
Monte-Carlo study with multivariable fit to the data from 3 cells of different size.



- 3 free parameters**
- rescale factor
 - upscattering scale
 - UCN elastic mfp

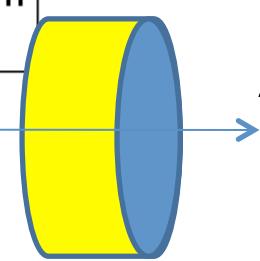
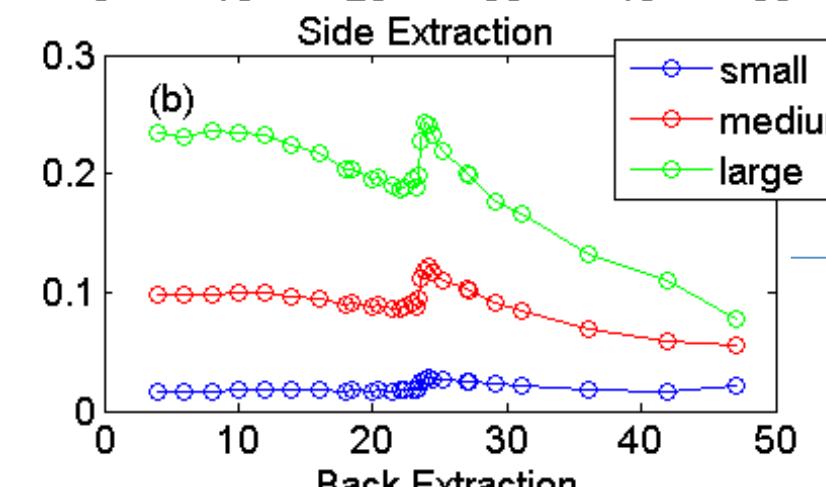


(UpScale: 1.9, CnMFP: 14 cm, σ_e : 0 b)

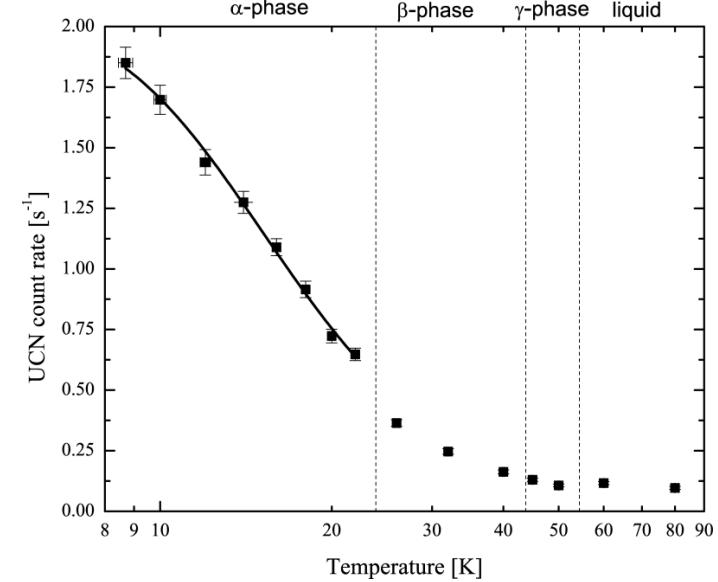
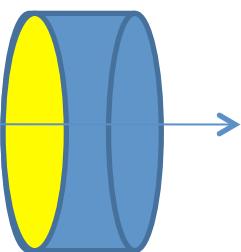
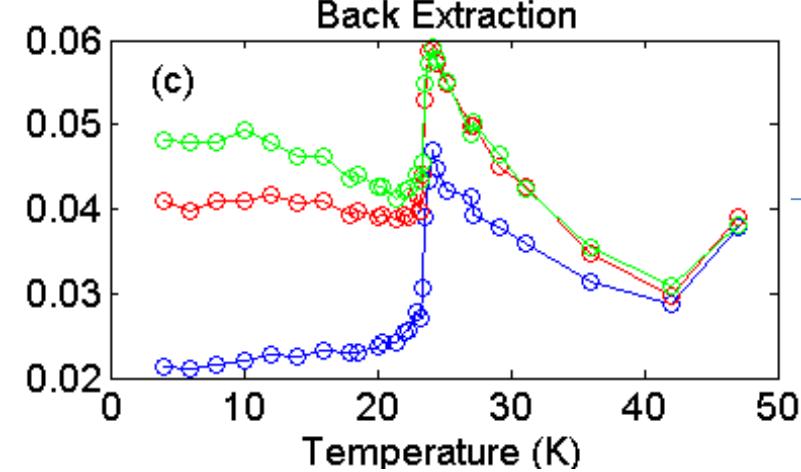


UCN Extraction

Yellow: extraction surface

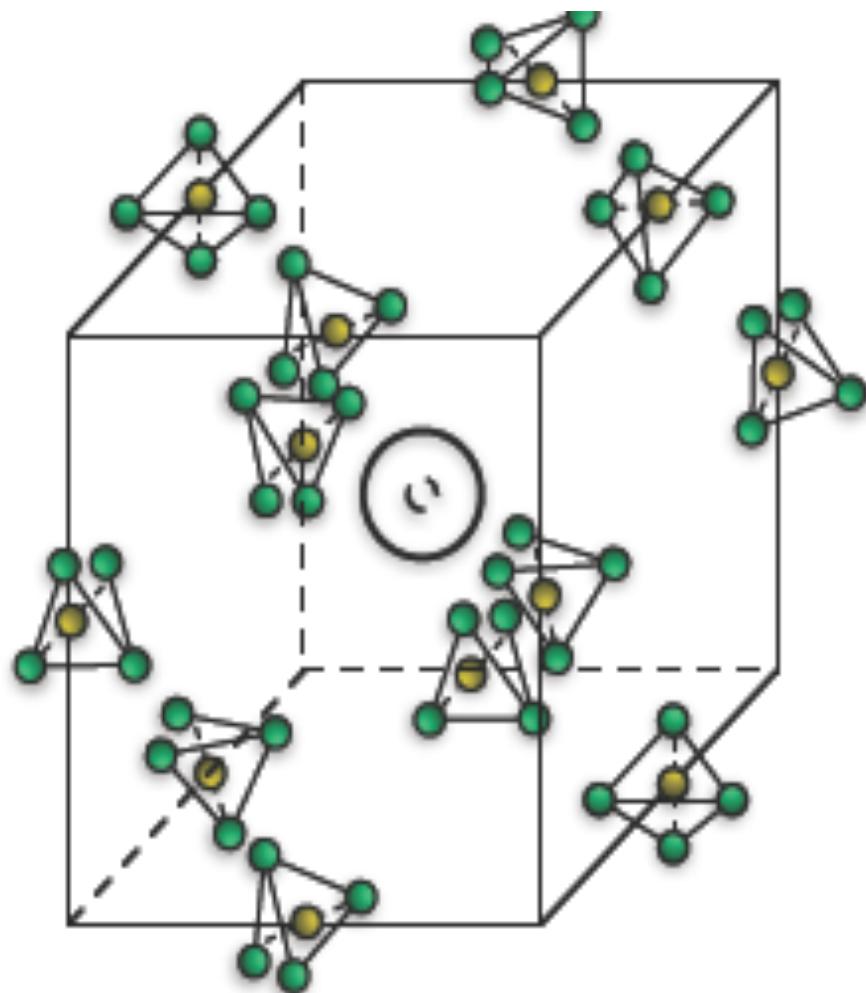


A. Frei et al., arXiv:1006.2970v1



Vertical extraction (side)¹⁸

Phase II Structure of Solid Methane

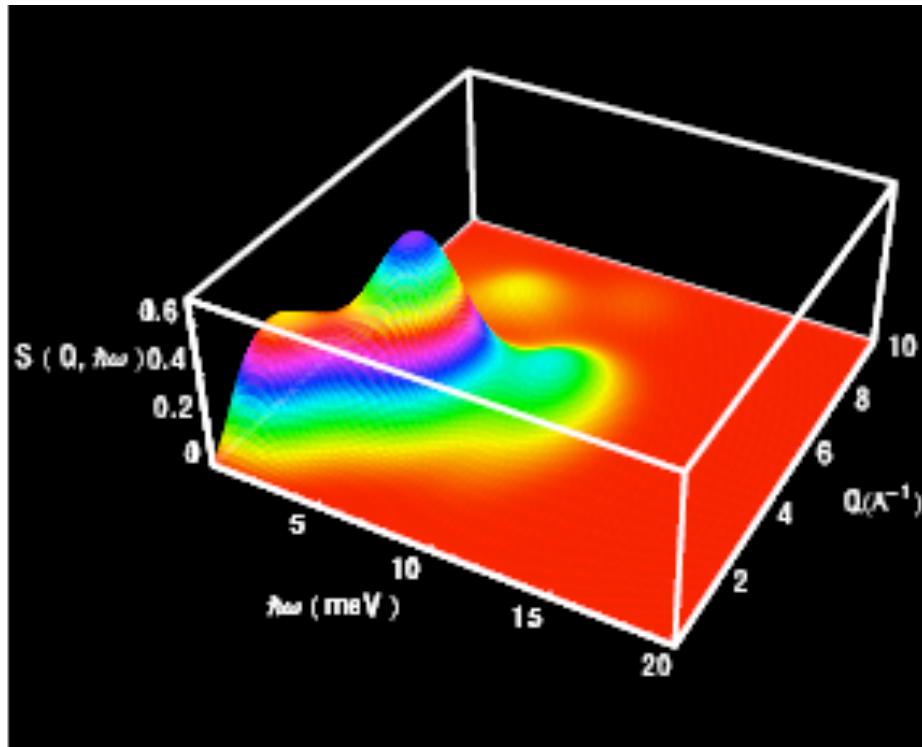


CH₄ is the brightest-known cold neutron moderator
(BUT not useable at high power sources due to rad damage)

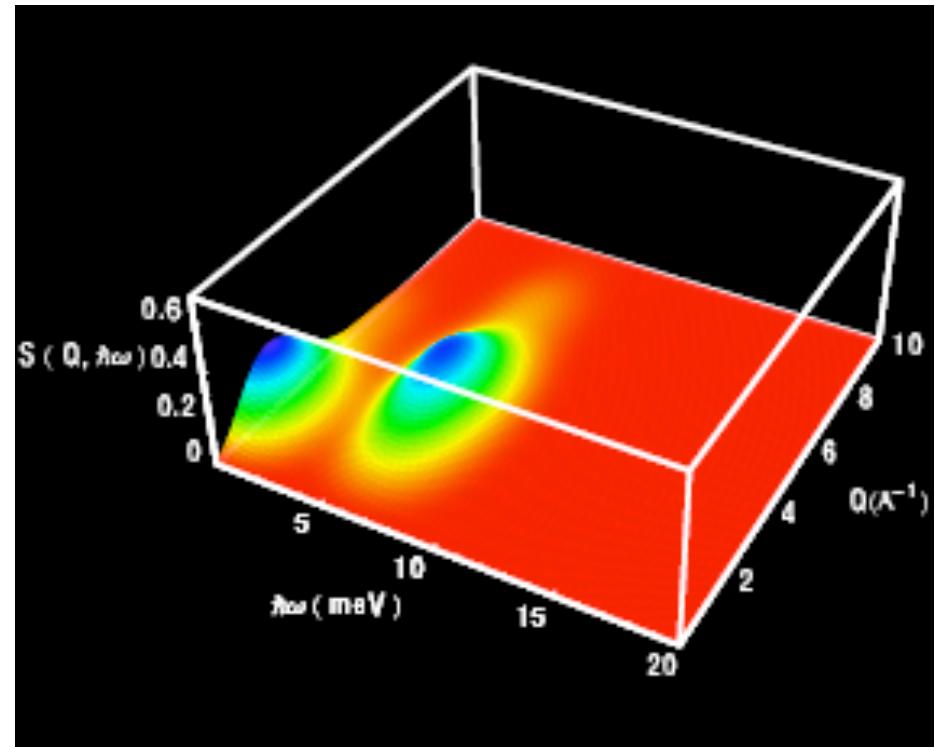
Below 20 K
 $\frac{1}{4}$ of the CH₄ are free rotors
 $\frac{3}{4}$ are hindered rotors

Above 20K
All sites are free rotors

$S(q,\omega)$ for CH₄



Free Rotational modes



Tunneling, Librational modes

Yun Shin developed a new MCNP kernel for CH₄ at various temperatures (including below 20K, in phase II) and used it with MCNP to reproduce the observed LENS n spectrum (in NIM)

Summary

- Need to expand the library of scattering kernels to optimize cold neutron sources.
- Take INS data (high resolution, CN + thermal) (+ total cross-section measurement) to streamline production of ENDF-VI files, needed for the above task.